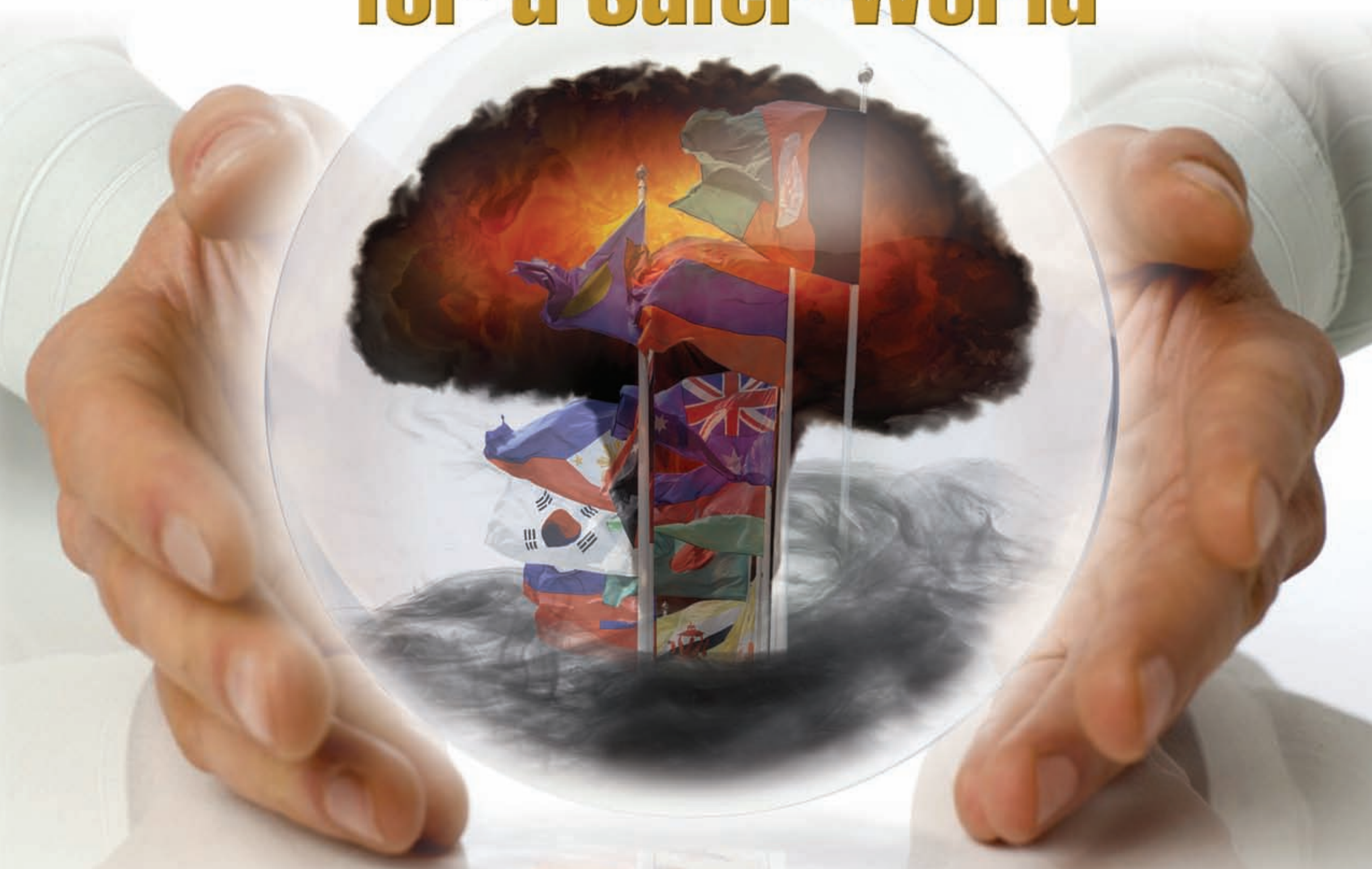
Lawrence Livermore National Laboratory

Science & Technology REVIEW

September 2010

Arms-Control Support for a Safer World



Also in this issue:

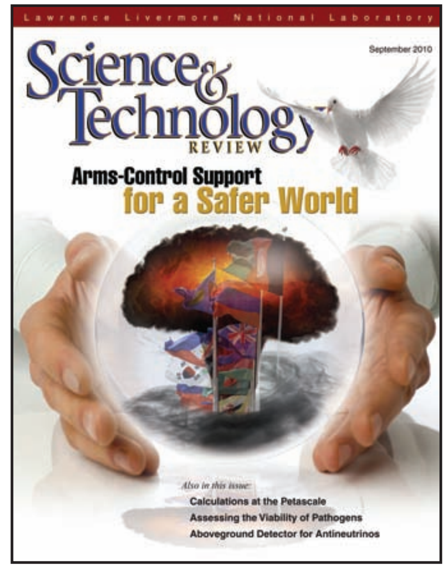
Calculations at the Petascale

Assessing the Viability of Pathogens

Aboveground Detector for Antineutrinos

About the Cover

The article beginning on p. 4 describes recent efforts by Lawrence Livermore in support of U.S. government agencies responsible for negotiating and implementing treaties that limit or ban weapons of mass destruction. Laboratory personnel have provided technical guidance on treaty conditions, analyzed the potential effects on national security, and contributed expertise on nuclear weapons and nonproliferation technologies to help the relevant governing bodies verify compliance. The artist's concept on the cover shows flags flying outside the Vienna International Center in Austria, superimposed on a rendering of a mushroom cloud from a nuclear weapon detonation. The center houses the International Atomic Energy Agency, which is responsible for verifying the peaceful uses of nuclear energy, and the Preparatory Commission for the Comprehensive Nuclear-Test-Ban Treaty Organization.



Cover design: George A. Kitrinos

About *S&TR*

At Lawrence Livermore National Laboratory, we focus on science and technology research to ensure our nation's security. We also apply that expertise to solve other important national problems in energy, bioscience, and the environment. *Science & Technology Review* is published eight times a year to communicate, to a broad audience, the Laboratory's scientific and technological accomplishments in fulfilling its primary missions. The publication's goal is to help readers understand these accomplishments and appreciate their value to the individual citizen, the nation, and the world.

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Please address any correspondence (including name and address changes) to *S&TR*, Mail Stop L-664, Lawrence Livermore National Laboratory, P.O. Box 808, Livermore, California 94551, or telephone (925) 423-3432. Our e-mail address is str-mail@llnl.gov. *S&TR* is available on the Web at str.llnl.gov.

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Contents

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Managing Editor
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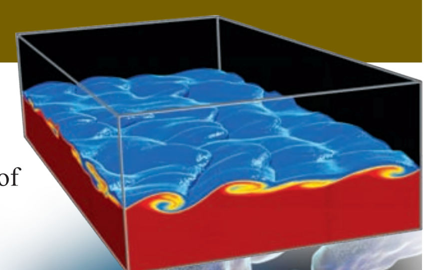
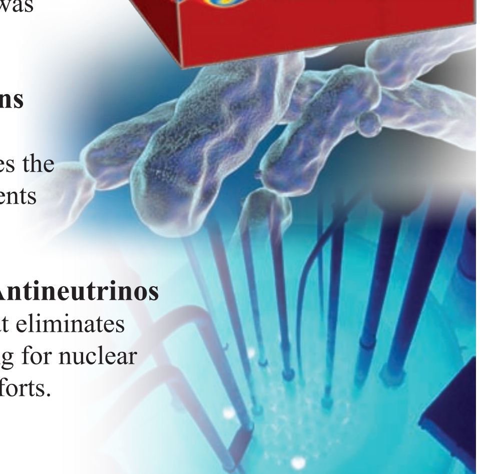
Feature

Research Highlights





Departments

Laboratory Captures Six R&D 100 Awards

Six technologies developed by teams of Livermore scientists and engineers and their collaborators have been honored with R&D 100 awards in *R&D Magazine*'s annual competition for the top industrial inventions worldwide. The winning technologies are as follows:

• GATOR, the grating-actuated transient optical recorder, is designed to acquire sequential images of x rays or optical light in a trillionth of a second or faster during experiments at the National Ignition Facility.

• The high-performance strontium iodide scintillator for gamma-ray spectroscopy is designed to use a new material, strontium iodide doped with europium, in radiation detectors to identify nuclear materials for homeland security and other important applications.

• Using microelectromechanical-systems-based adaptive-optics optical coherence tomography, ophthalmologists can view the eye's retina at the individual cell level, allowing them to diagnose retinal diseases at early stages and follow the progression of a disease and its treatment.

• SRaDS, the statistical radiation detection system, is a software application that nonexperts can use to rapidly and accurately distinguish nuclear materials, such as plutonium and uranium, from other radioactive substances.

• Ultrapermeable carbon nanotube membranes provide a filtration tool that separates ionic compounds such as salt from seawater or brackish water and can reclaim wastewater for use in crop irrigation and manufacturing processes.

• The x-ray free electron laser (XFEL) energy monitor measures the pulse-by-pulse energy of a photon beam emitted by an XFEL without being damaged by the beam or affecting beam quality.

With this year's results, the Laboratory has now captured 135 R&D 100 awards since 1978. The October/November issue of *S&TR* will highlight these award-winning inventions and the researchers who developed them.

Contact: Erik J. Stenehjem (925) 423-9353 (stenehjem1@llnl.gov).

Quantum Simulations Reveal Hydrogen's Transitions

Using quantum simulations, scientists from Lawrence Livermore, the University of Illinois at Urbana-Champaign, and the University of L'Aquila in Italy have examined the phase transitions of hydrogen under high pressure. Hydrogen is the most abundant element in the universe and a major component of giant gas planets, such as Jupiter and Saturn. However, much remains unknown about the transformation of hydrogen from one state to another. Results from this collaboration may help scientists understand how planets form.

The researchers discovered a first-order phase transition—a discontinuity—in liquid hydrogen between a molecular state with low conductivity and a highly conductive atomic state. Using the

temperature dependence of this discontinuity, they estimate that the critical point of the transition occurs at a temperature near 2,000 kelvins and pressure near 120 gigapascals. In addition, the hydrogen phase diagram produced by the simulations indicates that a multiphase coexistence point for liquid–liquid–solid hydrogen corresponds to the intersection of the liquid–liquid phase boundary. The team's research was published in the July 20, 2010, issue of *Proceedings of the National Academy of Sciences*.

Contact: Eric Schwegler (925) 424-3098 (schwegler1@llnl.gov).

A Close Look at Catalysts for New Energy Research

A new imaging technique on Livermore's dynamic transmission electron microscope (DTEM) has allowed scientists to observe the inner mechanisms of catalyst nanoparticles 3,000 times smaller than a human hair in nanosecond (billionth-of-a-second) increments. Their findings could greatly improve the efficiency of catalysts used in various processes that are crucial to the world's energy security, such as petroleum catalysis and catalyst-based nanomaterial growth for next-generation rechargeable batteries.

Scientists have achieved unprecedented spatial and temporal resolution in DTEM snapshots of nanoparticulate catalysts. The microscope's laser-driven photocathode can record short pulses of electrons with exposure times of 15 nanoseconds. An annular dark field aperture recently added to DTEM greatly improves its ability to time-resolve images of particles as small as 30 nanometers in diameter. Without the aperture, particle sizes were limited to 50 nanometers.

With the new technique, researchers can more easily discern significant features than they can with bright-field pulsed imaging technologies. DTEM images also have a temporal resolution that is six orders of magnitude higher than that of images taken with a conventional transmission electron microscope, revealing processes such as phase transformations, chemical reactions, and nanowire and nanotube growth. Results from the team's research appeared in the July 12, 2010, issue of *ChemPhysChem*.

Contact: Bryan Reed (925) 423-3617 (reed12@llnl.gov).

Commentary by Penrose (Parney) C. Albright

Toward a New Era of Global Security

On April 5, 2009, in a speech at Hradcany Square in Prague, Czech Republic, President Barack Obama set out his agenda for reducing global nuclear dangers and increasing U.S. national security. The subsequent Nuclear Posture Review, released in April 2010, provides a national security road map for preventing nuclear proliferation and terrorism while working toward the long-term goal of reducing the role and number of nuclear weapons.

International leaders have worked to prevent the spread of nuclear weapons at the state level by negotiating treaties that limit or ban such weapons and by securing weapons-usable nuclear materials. As described in the article beginning on p. 4, Livermore scientists have contributed to various arms-control agreements and treaties concerning nuclear nonproliferation, strategic force levels, and nuclear testing. Our technical expertise is directed not only toward protecting national security interests but also toward developing technologies to verify compliance with a treaty's terms and obligations. Livermore experts also help interpret the data collected in support of compliance judgments and enforcement.

For much of the Laboratory's existence, the consuming national security focus was monitoring and countering the nuclear arsenal of the Soviet Union. However, that world no longer exists. Today, with the rapid globalization of communication, transportation, and information networks, a determined adversary, a nation or even an individual acting alone, could deploy weapons of mass destruction (WMD) to wreak enormous damage on the U.S. To counter the latter threat, government agencies also pursue initiatives and agreements to prevent terrorism by nonstate actors.

The Laboratory has responded accordingly, extending its WMD expertise to chemical and biological weapons. We are one of two U.S. laboratories certified by the Organisation for the Prohibition of Chemical Weapons to analyze samples under the verification regime for the Chemical Weapons Convention. Our scientists are also advancing technology to more quickly identify biological threats, as described in the highlight beginning on p. 16.

International cooperation continues to grow in other technology-dependent areas such as public health and early detection of possible threats, providing more opportunities for our workforce to contribute to national security. In addition, treaty regimes being considered for space and cybersecurity would require tackling an entirely new set of technical issues and developing effective verification measures.

Another area of concern is the threat posed by nuclear proliferation. Livermore contributions to address this problem include research to advance tools that monitor WMD materials, technology, and expertise as well as processes that secure or eliminate inventories of materials and infrastructure used for those weapons. For example, the highlight beginning on p. 20 describes work to further improve antineutrino detectors so they can be deployed aboveground to monitor nuclear reactors.

A growing number of diplomats, scholars, and scientists, including Livermore researchers, are participating in discussions for Cooperative Threat Reduction 2.0, a U.S. initiative focused on building regional international partnerships to counter the threat of WMD proliferation. The aim of this initiative is to embrace multinational, regional projects that involve experts outside the defense and homeland security communities, such as the Departments of Agriculture and Health and Human Services, Centers for Disease Control and Prevention, Environmental Protection Agency, and federal law-enforcement agencies as well as academia, industry, and nongovernmental organizations. Clearly, the desired outcomes vary from country to country and from region to region—the threats in sub-Saharan Africa are vastly different from those in Southern Asia. The methods applied to achieve those goals must likewise be adapted to local institutions.

The long-term goal in all of these efforts is to make the world safer by promulgating safety and security standards where legitimate but potentially dangerous activities are occurring, by improving the transparency of activities in the relevant scientific communities, and by increasing the probability that nascent efforts to develop or proliferate WMD will be detected. From forging the unambiguous wording of a treaty to developing the tools to verify adherence to that treaty and providing federal agencies with the expertise needed to curb weapons and materials of mass destruction, Livermore personnel are dedicated to continuing their long-standing role in supporting arms-control and threat-reduction treaties.

■ Penrose (Parney) C. Albright is principal associate director for Global Security.

Science in Support of International Weapon Treaties

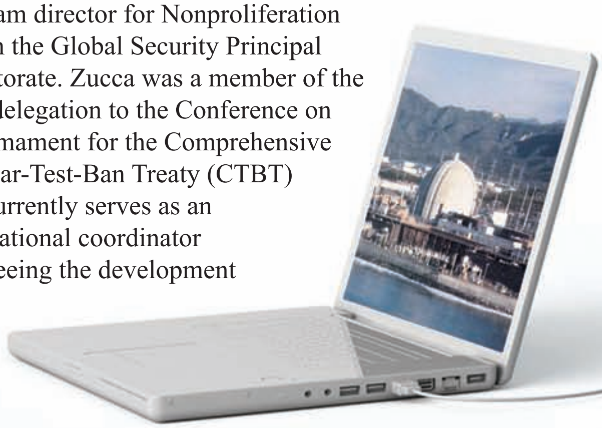
Livermore scientists provide technical expertise for negotiating and verifying treaties that limit or ban weapons of mass destruction.

FOUNDED as a nuclear weapons laboratory, Lawrence Livermore has for more than five decades helped support international treaties and agreements that limit or ban weapons of mass destruction. Laboratory experts have provided technical guidance for proposed treaties and have analyzed the possible effects of a treaty's provisions on national security. After a treaty enters into force, Livermore expertise about weapons, nuclear materials, and verification technologies contributes to U.S. and international efforts to ensure worldwide compliance with the treaty's terms and commitments. Indeed, the strength of treaties and arms reduction agreements rests, in large part, on the technical capabilities available for monitoring compliance.

"Laboratory employees have been involved at various levels with many international and bilateral treaties governing weapons of mass destruction," says Laboratory seismologist Jay Zucca, program director for Nonproliferation within the Global Security Principal Directorate. Zucca was a member of the U.S. delegation to the Conference on Disarmament for the Comprehensive Nuclear-Test-Ban Treaty (CTBT) and currently serves as an international coordinator overseeing the development of the International Monitoring System for the Preparatory Commission for the Comprehensive Nuclear-Test-Ban Treaty Organization in Vienna, Austria.

CTBT prohibits all nuclear explosions, including those intended for peaceful purposes. Dozens of Laboratory scientists worked for more than three decades providing technical support to U.S. government efforts to achieve this international agreement, which was signed by President Bill Clinton and other heads of state on September 24, 1996, at the United Nations. In signing the treaty, President Clinton used the same pen President John F. Kennedy had used to sign the Limited Test Ban Treaty in 1963. Clinton described CTBT as the "longest sought, hardest fought prize in the history of arms control negotiations."

Although 153 nations have ratified the pact, the treaty specifies 44 nuclear-capable states that must ratify CTBT before it can take effect. Of the 44,



nine have not ratified: the U.S., China, Indonesia, Egypt, India, Iran, Israel, Democratic People's Republic of Korea (North Korea), and Pakistan. India, Pakistan, and North Korea have conducted nuclear tests since CTBT was signed. Although the Senate has not ratified the treaty, the U.S. has not conducted a nuclear test since 1992. President Barack Obama has said he will "aggressively" push for CTBT ratification. (See the box on p. 7.)

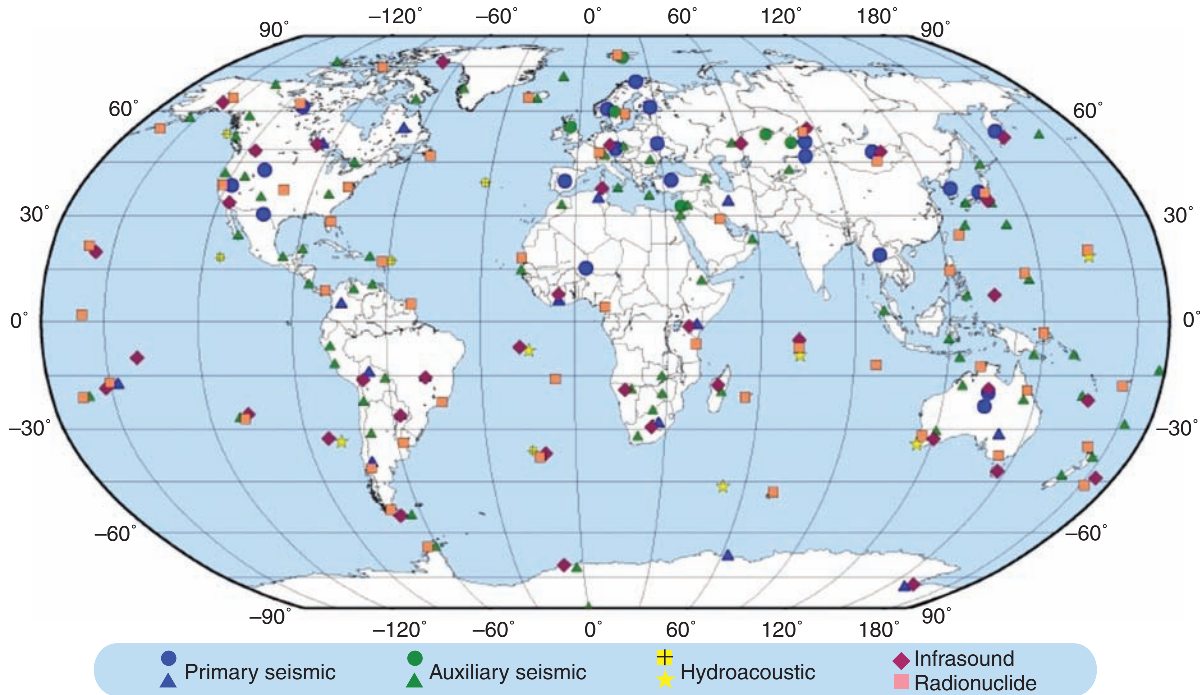
"Listening" to the World

CTBT's International Monitoring System is designed to search for evidence of clandestine nuclear explosions. In Vienna, an International Data Center processes data from hundreds of monitoring stations around the world. Although the network of stations is still in the buildup phase and is operating in testing and evaluation mode, it transmits data daily to the Vienna center. When complete, the International Monitoring System will have 321 stations and 16 laboratories located worldwide, including 50 primary and 120 auxiliary stations to monitor local seismic signals. In addition, hydroacoustic stations "listen" to the oceans, infrasound stations record very-low-frequency atmospheric sound waves, and radionuclide stations collect air samples to detect radioactive debris from atmospheric or underwater nuclear explosions as well as noble gases that could be produced by underground nuclear explosions.

During the 1990s, Livermore experts contributed to the CTBT negotiations in Geneva, Switzerland, by helping to select sites for monitoring stations, define procedures for onsite inspections, and adopt concepts for national monitoring. Since the treaty signing, Livermore researchers have worked on several Department of Energy projects that support the U.S. National Data Center at Patrick Air Force Base in Florida, the U.S. facility responsible for treaty monitoring. Bill Walter leads a team of about a dozen seismologists and other scientists in this effort. (See *S&TR*, March 2009, pp. 4–12.) The Laboratory is also working closely with the International Data Center to ensure an effective monitoring capability.

In a National Geographic Explorer documentary, "Inside the Nuclear Threat," which first aired in April 2010, Zucca discusses how seismology can detect underground nuclear tests. "Many events, such as a small earthquake, can produce a seismic signature similar to a small clandestine nuclear detonation," he says. Every year, more than 200,000 earthquakes occurring around the world have a similar seismic magnitude to that of a small underground nuclear explosion. Laboratory researchers are pioneering methods to more accurately distinguish a nuclear explosion from other seismic events, including earthquakes, volcanoes, and mining activity, and to pinpoint

Livermore scientists provide technical expertise in support of international efforts to limit or ban nuclear weapons. Many Laboratory technologies are used to monitor compliance with a treaty's provisions. Examples (shown in the computer screens from left) include detectors for monitoring nuclear power plants, new materials for detecting radiation, and forensic seismology tools for distinguishing earthquakes and other seismic disturbances from underground nuclear explosions.



The International Monitoring System for the Comprehensive Nuclear-Test-Ban Treaty searches for evidence of clandestine nuclear explosions. When complete, the system will comprise 321 seismic, hydroacoustic, infrasound, and radionuclide stations and 16 laboratories worldwide. (Courtesy of Preparatory Commission for the Comprehensive Nuclear-Test-Ban Treaty Organization.)

The Vienna International Centre in Vienna, Austria, houses the International Atomic Energy Agency (IAEA) and the Preparatory Commission for the Comprehensive Nuclear-Test-Ban Treaty Organization. (Courtesy of IAEA; photographer: Dean Calma.)

an event's location. They are also working with scientists throughout the Middle East and Asia to determine how regional geology affects seismic signals, which travel underground before being recorded.

When India and Pakistan conducted underground nuclear tests in 1999, Livermore scientists used seismic data recorded from the blasts to successfully differentiate the nuclear tests from typical regional earthquakes. In the process, they characterized the test yields and noted inconsistencies between the announced yields and the inferred results. The signals from the nuclear tests also provided important data for calibrating seismic stations in this geologically complex region.

When North Korea declared it had conducted a small nuclear test in October 2006, only two-thirds of the 321 seismic stations for the International Monitoring System had been installed. Nevertheless, the system performed extremely well, with 22 stations detecting the low-yield explosion. On May 25, 2009, North Korea announced another nuclear test. At that time, about 85 percent of the monitoring system had been installed, and 61 stations recorded the event. The extensive data set permitted a more precise assessment of the event's location and magnitude. The following month, Laboratory personnel were among the 500 verification technology experts from 86 countries who gathered in Vienna for the International Scientific Studies Conference to discuss the treaty's capabilities to detect nuclear explosions in light of the two North Korean tests.

An important element of CTBT is the provision for an onsite inspection, which may be requested when remote systems cannot resolve the nature of a suspicious event. A group of inspectors will then search the area identified as the possible nuclear-test location. Livermore experts have led the development of onsite inspection technologies and procedures, such as looking for underground explosion cavities or rubble. Laboratory-developed tools also can detect small amounts of the rare radioactive gases that would be generated by an underground nuclear detonation and then would migrate to the surface. In addition, three Laboratory scientists serve on the five-member inspection team for the U.S.

Safeguards to Prevent Proliferation

Preventing the spread of nuclear weapons requires efforts on many fronts. Monitoring activities provide evidence to verify that no nuclear experiments are conducted and that no nuclear materials are stolen, diverted, or clandestinely produced. In addition, controls are needed to prevent the export of nuclear facilities, equipment, and sensitive technology.

The International Atomic Energy Agency (IAEA) is responsible for verifying peaceful uses of nuclear energy under the Nuclear Non-Proliferation Treaty. Established in 1957 as the world's "Atoms for Peace" organization, IAEA implements various verification measures (safeguards) to ensure that nuclear facilities and materials are not misused for military purposes. The Nuclear Non-Proliferation Treaty, which limits the spread of nuclear weapons, came into force in 1970 and has been ratified by 189 states. (India, Pakistan, and Israel have not signed or ratified the treaty. North Korea ratified it in 1985 but withdrew from participation in 2003.)

The treaty requires a participating nonnuclear weapon state to sign a comprehensive safeguards agreement with IAEA and to place all of the state's nuclear material and activities under IAEA safeguards. The agency regularly inspects nuclear facilities in 57 nonnuclear weapon countries. Inspectors confirm nuclear material inventories, review surveillance camera footage, analyze environmental samples, and look for evidence of undeclared activities.

The Laboratory supports IAEA's nuclear safeguards mission by developing new technologies and providing expert advice to the agency and to U.S. policy makers. Livermore personnel not only work with international partners to strengthen safeguards implementation but also take leaves of absence to serve as IAEA staff members. Laboratory scientists Tony Lavietes and Cynthia Annese are currently working at the IAEA Department of Safeguards in Vienna. Researchers Young Ham, Jonathan Essner, and George Anzelon have also worked there in years past.

Livermore scientists have developed both portable and stationary tools to detect and characterize materials produced as part of the nuclear fuel cycle. One example is GeMini, a handheld high-resolution gamma spectrometer developed by a team led by physicist Morgan Burks. (See

Nuclear Arms Treaties Nearly as Old as Nuclear Weapons

Since the first experiment with a nuclear explosive was conducted in 1945, a succession of treaties has narrowed the lawful environment for nuclear testing. Public concern over atmospheric testing led the U.S. and the Soviet Union to establish a Conference of Experts to examine the technical issues associated with a comprehensive ban on nuclear weapons testing in all environments, including the atmosphere, outer space, underwater, and underground. Ernest O. Lawrence, the Laboratory's cofounder, served as one of three U.S. representatives to this conference. Harold Brown, who became Laboratory director in 1960, was a member of the delegation's technical advisory group.

At the end of the conference in 1958, the U.S. and the Soviet Union entered into a nuclear testing moratorium, and negotiations began on a test-ban treaty. Livermore scientists participated in technical working groups complementing the negotiations on a comprehensive nuclear test ban. Measuring seismic signals was considered a viable technique for detecting underground explosions, and a worldwide network of seismic stations was built as part of this effort. The Soviet Union's resumption of nuclear testing in September 1961 broke the bilateral moratorium and ended the negotiations at that time.

In the ensuing decades, the Laboratory contributed to arms-control negotiations on strategic force levels and nuclear testing. These negotiations led to a number of successful international treaties. The Limited Test Ban Treaty, ratified in 1963, banned nuclear explosions in the air, oceans, and space. President Richard Nixon and Soviet Secretary Leonid Brezhnev signed the Threshold Test Ban Treaty in 1974, although the U.S. Senate did not ratify it until 1990. That treaty limited underground nuclear tests to 150 kilotons. By comparison, the bomb dropped on Hiroshima had a yield of 15 kilotons.

The Comprehensive Nuclear-Test-Ban Treaty was signed in 1996, following many years of negotiations. It prohibits all nuclear explosions but has yet to be ratified by the U.S. Senate.

The Strategic Arms Reduction Treaty (START), a bilateral treaty between the U.S. and the Soviet Union, was signed in 1991. It succeeded the Strategic Arms Limitation Treaty I and II, agreed to in the 1970s. Shortly after signing START, the Soviet Union dissolved. Negotiations continued with the former Soviet republics, allowing START to enter into force in 1994. START barred its signatories from deploying more than 6,000 nuclear warheads atop a total of 1,600 intercontinental ballistic missiles, submarine-launched ballistic missiles, and bombers. The treaty expired in December 2009.

New START, signed in 2010 by U.S. President Barack Obama and Russian President Dmitry Medvedev, reduces strategic delivery vehicles by more than half and deployed warheads by three-quarters compared with the START limits. This agreement will enter into force after the two countries' legislatures ratify it.

Directors from the National Nuclear Security Administration's three weapons laboratories testified in July 2010 before the Senate Armed Services and Foreign Relations committees on the prospects for sustaining the nation's nuclear stockpile under New START. Lawrence Livermore Director George Miller noted that the Stockpile Stewardship Program is "a cornerstone of the nation's strategic deterrent for the future" and emphasized the continued need for a stewardship program that is "balanced, integrated, and sustained over time."

Laboratory researcher Young Ham (center) and two South Korean scientists prepare to test a prototype of a Livermore-developed spent-fuel verification instrument at the Kori-2 nuclear power station in Gori, Republic of Korea.

In July 1991, Livermore physicist Jay Davis, who later served as an associate director, worked on an IAEA inspection team in Iraq. This photo shows Davis examining the bombed remains of Iraq's clandestine uranium enrichment facility at Al Tarmiyah. (Courtesy of IAEA.)

S&TR, October/November 2009, pp. 8–9.) An R&D 100 Award–winning technology, GeMini does not need liquid nitrogen for cooling and thus can be used in the field to accurately identify nuclear materials. A version is being built for the international safeguards community to evaluate for use in IAEA inspections at nuclear facilities and other locations.

Another promising technology for safeguarding nuclear facilities is the liquid scintillator multiplicity counter being designed by researchers from Lawrence Livermore and Sandia national laboratories. (See *S&TR*, July/August 2008, pp. 23–25, and the highlight beginning on p. 20.) In addition, Ham leads a team developing innovative methods to verify spent fuel stored at reactor sites, in cooperation with the Republic of Korea and other nations. Another team, led by researcher Faranak Nekoogar, is developing ultrawideband radio-frequency identification tags for tracking nuclear material containers.

Lawrence Livermore is also a member of IAEA's Network of Analytical Laboratories. In this role, Ross Williams and his team of chemists analyze a portion of the environmental samples collected by IAEA during its inspection activities and report results back to IAEA. The Laboratory also conducts research to develop analytical techniques and methods for interpreting safeguards-relevant signatures present in these samples.

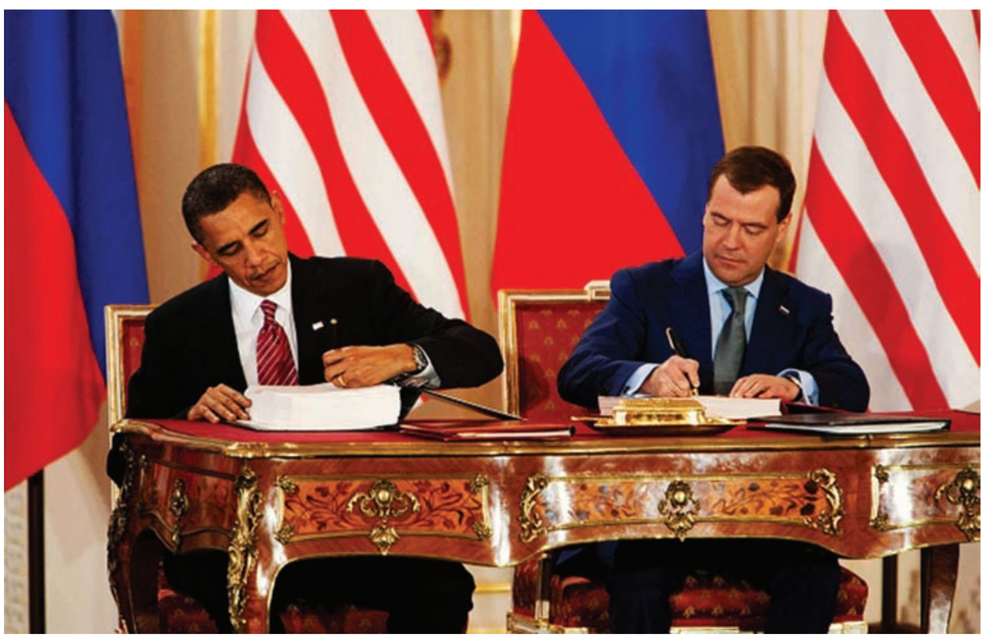
Expertise for Inspections

In a few special cases—notably Iraq, Libya, and North Korea—countries have agreed, either voluntarily or under the threat of action from the United Nations' Security Council, to disclose and eliminate previously clandestine nuclear capabilities. To support this effort, several DOE laboratories, including Lawrence Livermore, have provided experts to work with or in parallel to IAEA's expert teams. For example, following the 1991 Gulf War, Livermore's Anzelon, Bill Nelson, Jay Davis, Lee McLean, Ron Kerst, Bill Domke, Bill Conaway, Frank Pabian, Jackie Kenneally, Cal Woods, and Bill Quirk participated in IAEA inspection teams that uncovered and dismantled Iraq's secret nuclear weapons program. In early 2003, Domke and Rob Schmidt served on IAEA teams inspecting Iraq in the weeks before the second Gulf War. Heather Harvey and Jennifer Swenson joined Domke and Kerst as participants in the U.S. inspection following that war.

Libya agreed to disclose its formerly secret nuclear program in 2004 and allowed the U.S. and the United Kingdom to remove sensitive nuclear equipment and materials. Mark Franks, an engineer at the National Ignition Facility, contributed to plans for the removal operation. Other Livermore staff traveled to Libya to help inspect facilities, remove equipment, and verify activities. More recently, as part of the now-moribund denuclearization efforts in North Korea, the Department of Energy and several of its laboratories sent personnel to monitor disablement activities at the Yongbyon nuclear center. Livermore's Lisa Szytel, now with the National Nuclear Security Administration, led several monitoring teams in North Korea. Another Laboratory scientist led the nuclear monitoring team that was expelled, along with IAEA monitors, in April 2009 when North Korea abrogated its denuclearization agreement.

To help strengthen IAEA verification technologies and scientific resources, DOE launched the Next Generation Safeguards

In 2004, Livermore scientists assisted a U.S.—United Kingdom effort to remove large quantities of sensitive nuclear materials and nuclear material processing equipment from Libya. In this photograph, U.S. personnel are positioning a container of uranium hexafluoride in a cargo aircraft prior to departure from Libya. (Courtesy of U.S. Department of Energy.)



U.S. President Barack Obama (left) and Russian President Dmitry Medvedev signed the New Strategic Arms Reduction Treaty (New START) on April 8, 2010, in Prague, Czech Republic. (Courtesy of U.S. Department of State and White House; photographer: Chuck Kennedy.)

U.S. and Russian delegations sat opposite one another at the New START negotiating table in Geneva, Switzerland. (Courtesy of U.S. Department of State; photographer: Eric Bridiers.)

Initiative in 2009. Mona Dreicer, the deputy program director for Nonproliferation, supported colleagues at the National Nuclear Security Administration's Office of Nonproliferation and International Security to develop the initiative's implementation plan. To help train the next generation of safeguards professionals, the Laboratory and the Monterey Institute of International Studies prepared a short course on safeguards policy and information analysis. Many Livermore researchers also mentor graduate students assigned to safeguards-related projects.

New START for Disarmament

Because they have first-hand knowledge of nuclear weapons, radiation detection capabilities, and verification technologies, Livermore researchers have worked on many nuclear treaty negotiations. Dreicer supported DOE as part of the U.S. delegation at negotiations for the follow-on agreement to the Strategic Arms Reduction Treaty (or New START) between the U.S. and Russia. The original START agreement, which was signed in 1991 and expired in 2009, dramatically reduced the number of strategic delivery systems and deployable warheads for both countries.

U.S. President Obama and Russian President Dmitry Medvedev signed New START on April 8, 2010. The agreement will cut American and Russian deployed strategic nuclear warheads to 1,550 over seven years, about a third less than the 2,200 warhead limit established in 2002 under the Moscow Treaty. In comparison, the U.S. deployed about 19,000 warheads at the end of the Cold War. Within the next seven years, both nations will reduce their total land-, sea-, and air-based launchers to 800, with no more than 700 deployed intercontinental and sea-launched ballistic missiles and heavy bombers. New START is awaiting ratification by the U.S. Senate and the Russian Duma.

Dreicer's background includes modeling radionuclides and determining their effects on people and the environment. Her work, which has involved evaluating health and environmental impacts of the 1986 accident at the Chernobyl nuclear power plant, brought her to the U.S. Arms Control and Disarmament Agency as a technical expert on the radionuclide monitoring network for CTBT. When the agency became part of the State Department, her role expanded to leading the office that worked on verifying compliance with nuclear arms-control and nonproliferation agreements.

During the past year, in support of DOE, Dreicer participated in the Treaty Text Working Group of the New START Delegation in Geneva. This group was responsible for ensuring that the treaty articles accurately conveyed the terms agreed to by the Russian and American delegations. She also participated with the team responsible for developing the treaty's terms and definitions, a protocol

Negotiators present the details of New START to international arms-control diplomats at a plenary session of the 2010 Conference on Disarmament in Geneva, Switzerland. (Courtesy of U.S. Department of State; photographer: Eric Bridiers.)

section that applies to the treaty articles, protocol sections, and related documents.

Livermore radiochemist John Luke spent many months at DOE headquarters helping to develop negotiating positions for the U.S. government. Engineer Carolyn Pura from Sandia National Laboratories, California, supported DOE by contributing expertise to develop the treaty's inspection and telemetry components.

Dreicer notes that New START required less than a year of preparation—an extraordinarily short time. "For START I, we saw higher levels of mistrust on both sides," she says. "New START reflects the current state of improved relations between the U.S. and Russia."

A Ban on All Chemical Weapons

Unlike nuclear treaties that limit the numbers and types of permitted weapons, the Chemical Weapons Convention (CWC) bans an entire class of weapons of mass destruction. It outlaws the development, production, acquisition, stockpiling, and use of chemical weapons. Signatory nations must destroy any chemical weapon stockpiles and production facilities. The treaty also bans the transfer of chemical weapon–related technologies to other countries or groups. CWC is the first arms-control treaty to widely affect the private sector because many chemicals of concern have legitimate civilian uses. As a result, industrial facilities as well as government sites are subject to inspections.

CWC opened for signing in 1993 and has been ratified by 188 countries, including the U.S. The Organisation for the Prohibition of Chemical Weapons (OPCW), headquartered in The Hague, Netherlands, implements the treaty.

A unique feature of CWC is its incorporation of the "challenge inspection," whereby any signatory in doubt about another signatory's compliance can request that the OPCW Director-General send an inspection team. By agreeing to this procedure, signatories have committed to the principle of "anytime, anywhere" inspections with no right of refusal.

Livermore's work supporting OPCW is performed by the Forensic Science Center (FSC) as part of Global Security's Nonproliferation Program. FSC is one of 19 laboratories around the world certified by OPCW to support challenge inspections. The other certified U.S. laboratory is at the Army's Forensic Analytical Center at Edgewood Chemical Biological Center in Maryland. OPCW requires that samples from sites under challenge be analyzed by two OPCW-certified laboratories. U.S. legislation, however, requires that all samples collected in the U.S. be analyzed within the country. Thus, the U.S. needs two OPCW-certified laboratories to comply with the treaty.

Livermore was selected to be the nation's second OPCW-designated laboratory because its capabilities include chemical analysis and forensic

Livermore chemist Saphon Hok synthesizes a compound as part of the Forensic Science Center's annual recertification exercise for the Organisation for the Prohibition of Chemical Weapons.

characterization of unknown samples and detection of trace levels of unknown compounds. In addition, the Laboratory operates under strict environmental controls and tight physical security.

An OPCW-designated laboratory must be able to detect traces of tens of thousands of possible compounds, including chemical warfare agents, precursor chemicals, and decomposition products, often in the presence of other compounds that complicate the analysis. The laboratory must then synthesize the identified chemicals to verify the analysis and report the results—all within 15 days. "OPCW can call us any time to perform an analysis," says analytical chemist Armando Alcaraz.

All OPCW laboratories must be recertified every year, which requires passing a stringent proficiency test. Test samples typically contain mixtures of many compounds, some of which are added to deliberately mask an incriminating species. For example, facility operators who are clandestinely producing chemical weapons might dump chemicals on the ground near the production facility and then bleach the soil minutes before OPCW inspectors arrive. To ensure that certified laboratories can distinguish chemical warfare agents in those types of samples, OPCW might spike a test sample with bleach. Samples can be in many forms, from soil and decontamination products to aqueous solutions, organic reaction mixtures, and compounds that seem to be chemical agents but are not. Pesticides and their degradation products, in particular, can appear similar to chemical weapons.

FSC chemists use an array of analysis techniques, including mass spectrometry, gas chromatography, nuclear magnetic resonance, and Fourier transform infrared spectroscopy. However, successfully passing the annual recertification test requires far more than having sophisticated equipment. Critical tasks include carefully preparing the sample so its constituents can be identified, completing the analysis, interpreting data correctly, and reporting results to the proper authorities.

Obtaining certification in 2003 brought national recognition to the center and work from the Department of Homeland Security, Environmental Protection Agency (EPA), Food and Drug Administration, and Federal Bureau of Investigation. FSC scientists have led training workshops at various EPA laboratories, showing staff members how to analyze materials containing chemical weapon agents. In the event of a chemical attack at a busy public facility, such as an airport, EPA would then call on these laboratories to determine the extent of chemical agents in building materials such as drywall, floor tiles, and carpeting. Materials would be tested again, after decontamination efforts, to ensure that the facility could be safely reopened to the public. (See *S&TR*, March 2010, pp. 4–10.)

FSC is also certified to store and handle small quantities of nerve agents, so it routinely evaluates new detection instruments for the Department of Homeland Security and law-enforcement agencies. "Surrogates to the main chemical weapons exist, and we might use them in the initial development and testing phases," says Alcaraz. "But until we've tested a device on the real thing, we can't say with 100-percent confidence that it can detect a chemical agent."

National Security in Full Context

Throughout its history, the Laboratory has played a major role in ensuring the safety, security, and performance of the nation's nuclear deterrent, first through its historical work in designing and testing nuclear weapons and, since the early 1990s, through the nation's Stockpile Stewardship Program. Efforts in support of treaty negotiations and verification activities may be less well known. History may show, however, that this work has made an equally important contribution toward ensuring the nation's security.

—Arnie Heller

Key Words: Chemical Weapons Convention (CWC), Comprehensive Nuclear-Test-Ban Treaty (CTBT), Forensic Science Center (FSC), GeMini, International Atomic Energy Agency (IAEA), International Monitoring System, Limited Test Ban Treaty, New Strategic Arms Reduction Treaty (New START), Next Generation Safeguards Initiative, Nuclear Non-Proliferation Treaty, Organisation for the Prohibition of Chemical Weapons (OPCW), Threshold Test Ban Treaty.

For further information contact Jay Zucca (925) 422-4895 (zucca2@llnl.gov).

Crossing Computational Frontiers

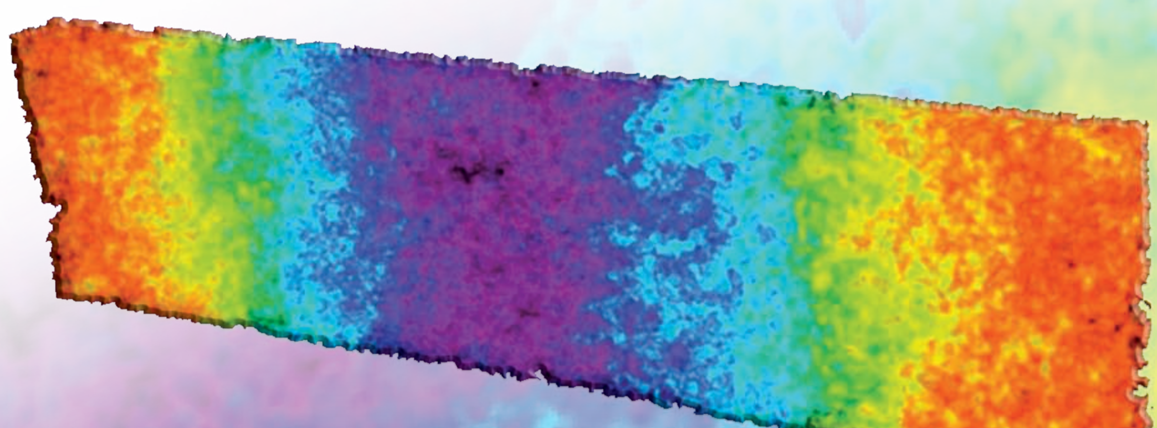
WHEN Dawn, Lawrence Livermore's latest supercomputer, was installed in 2009, scientists at the Institute for Scientific Computing Research (ISCR) were among the first to put it to work. In doing so, they demonstrated an innovative parallelization strategy for simulating at unprecedented resolution and scale the hot, dense plasmas that will occur during fast ignition, the implosion–explosion process to ignite a fusion reaction, at the National Ignition Facility. Their strategy helped solve one of the most difficult scaling problems in numerical simulation: the efficient parallel calculation of long-range interactions. Long-range forces (such as electrostatic or gravitational) are relevant to a variety of modeling scenarios. Previous efforts to develop a fully scalable solution to this complex calculation have failed on less powerful machines.

ISCR's mission is to assemble and maintain multidisciplinary teams of researchers who work with Livermore project specialists in designing computer applications that address program needs. The institute also collaborates with students and other guests to advance computational capabilities. (See the box on p. 14.) Teams choose test-bed projects to push the envelope of application performance on today's supercomputers. Through this work, ISCR is creating a scientific computing capability that supports the Laboratory's missions and is developing the technology and expertise needed to effectively utilize next-generation computers, which are expected to expand from thousands to millions of processors.

Computers keep getting larger and more powerful, and Livermore excels at maximizing their potential. "Big computers do not arrive as turnkey devices," says ISCR Director Fred Streitz, who also leads the modeling and simulations group in Livermore's Physical and Life Sciences Directorate. "To use these machines to their utmost, exploring more complex problems with ever-increasing resolution, scientists must rethink old approaches and devise new algorithms."

Streitz is quick to credit his team of computational specialists for the institute's success. He lauds team leader Jim Glosli and team members Bor Chan, Milo Dorr, Erik Draeger, Jean-Luc Fattebert, Liam Krauss, David Richards, Tom Spelce, and Michael Surh for their ingenuity and dedication in completing the fast-ignition simulation. "Computers run 24/7," says Streitz, "and the researchers operating these machines sometimes must do nearly the same."

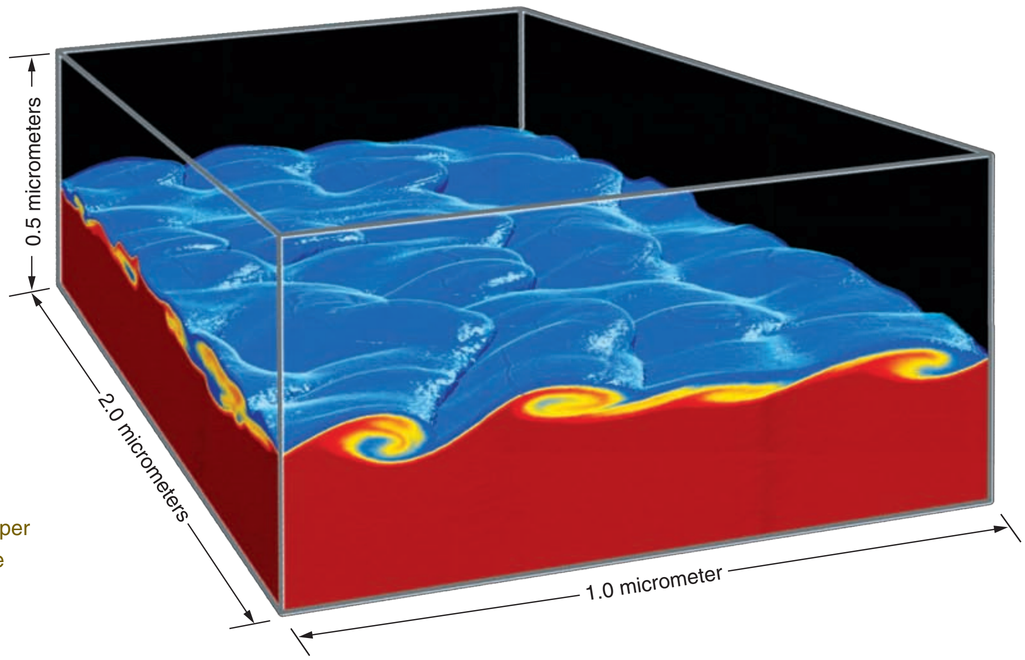
Glosli, Richards, and Streitz are veterans of a previous campaign, which ran for six continuous weeks and used the entire BlueGene/L supercomputer—more than 200,000 processors. In that



Even with the computational power of the Dawn supercomputer, researchers can simulate only a thin slice of hot, highly energized argon-doped deuterium–tritium plasma as it is heated by a proton beam. After the beam passes through the plasma, the center (purple) is the hottest region of the plasma, and temperatures drop away to the outer edges (red).

groundbreaking simulation, they modeled up to 62.5 billion atoms of liquid aluminum flowing across liquid copper. For their effort, they were honored with the 2007 Gordon Bell Prize and with the Laboratory Director's Science and Technology Award in 2008.

Between them, ISCR team members have earned eight Gordon Bell prizes over the past five years. Named for C. Gordon Bell, one of the founders of supercomputing, this prize annually recognizes outstanding achievement in high-performance computing, with an emphasis on rewarding innovative science applications. Bell established the prize in 1987 to encourage the further development of parallel processing, the computer design philosophy that has driven high-performance computing since the 1980s.



All of the processors on the giant BlueGene/L supercomputer ran for six weeks to produce this 1-cubic-micrometer simulation of liquid copper flowing like waves reaching a shore across liquid aluminum.

Hosting Visitors, Gaining Collaborators

The Institute for Scientific Computing Research (ISCR) manages an extensive visitor program for the Laboratory's Computation Directorate, hosting many guests and postdoctoral researchers throughout the year. For many years, outreach was the institute's primary goal, and it remains an important function. "We want our visiting students, postdocs, and faculty to be as actively involved in our projects as possible," says ISCR Director Fred Streitz.

Such collaborations expose students and faculty to the stimulating and challenging work environment of a national laboratory and generate considerable goodwill for Lawrence Livermore. Many students and postdoctoral researchers later join the Laboratory as staff researchers.

The institute's largest effort is the Summer Visitor Program, which this year brought 100 students and 20 faculty members to Livermore. In any one year, about half of the visitors might come from foreign countries, making logistics quite complicated. Faculty can arrange for sabbatical visits that last up to 12 months. ISCR also serves as the host to computer science graduate students whose academic program is funded through the Lawrence Scholar Program.

Candidates selected for the Summer Visitor Program are hired as summer employees and assigned to work with Laboratory mentors on specific projects. The nature of the project and the assigned work are chosen to complement each candidate's background and skills. Visits may last from 4 to 30 weeks (sometimes continuing into the fall semester). During that time, participants have an opportunity to learn more about their chosen field and related research areas through numerous seminars and informal interactions with staff and other visitors to the institute.

ISCR also provides opportunities for shorter-duration visits. Scientists and scholars from academia or industry often merit intermittent access to the Laboratory's staff and resources when funding is not the critical issue. Such arrangements allow visitors and ISCR scientists to explore research areas of mutual interest. According to Streitz, "Our administrative staff stays incredibly busy making arrangements for all these programs and various visitors."

A New Supercomputing Era

The Dawn supercomputer, which Streitz says is "shockingly powerful," comes from the same IBM lineage as BlueGene/L, which held the title of world's fastest supercomputer from November 2004 to May 2008. Dawn can perform 500 trillion floating-point operations per second (teraflops) and is laying the applications foundation for Sequoia, a 20-petaflops (or 20 quadrillion floating-point operations per second) machine scheduled for delivery in 2011.

Sequoia will process calculations designed to build more accurate physical models of nuclear weapon detonations and will strengthen predictive capabilities by running very large suites of complex simulations. This work is a cornerstone of the National Nuclear Security Administration's Stockpile Stewardship Program to ensure the safety, security, and effectiveness of the U.S. nuclear weapons stockpile without underground testing.

Improving Traffic Flow on the Processors

Igniting plasma to achieve fusion requires heating and compressing the target fuel to extremely high temperatures and pressures. To achieve ignition conditions, researchers must understand and control the energy flow in and out of the laser system as well as between various plasma components, such as ions, electrons, and photons. A direct particle simulation of inhomogeneous nonequilibrium plasma can capture the many-body physics of the energy flow and provide that understanding, but the calculation is computationally challenging. The key hurdle—deemed impossible by some—is developing efficient methods to scale the routines that solve for the effect of long-range Coulomb forces so these mechanisms can be simulated at the relevant sizes.

Students (from left) Daniel Osei-Kuffuor and Hilari Tiedeman work with Livermore scientist Rhys Ulerich as part of the annual Summer Visitor Program hosted by the Institute for Scientific Computing Research.

Impossible to some, but not for the ISCR team. In analyzing the problem, the researchers noted that the Coulomb solver has two main computational pieces that, although largely independent, have different scaling behaviors. This observation led them to develop a heterogeneous decomposition process so that scientists can flexibly map, or "tune," the computational pieces to subsets of the hardware. The tunable approach provided excellent scaling of the Coulomb problem to thousands of processors. As a result, computational experts can for the first time incorporate long-range physics into extremely large-scale simulations.

Think of driving down a winding, two-lane road. No matter how fast you want to drive, the slowest car determines the speed for all cars in your lane. Computer scientists faced this problem in extending sequential applications to calculate complex interactions. Solving that problem led to parallel computing, which is like adding more lanes to the highway.

Even with today's massively parallel technology, the analogy still applies. "Using a single strategy to parallelize a simulation limits overall scalability because the least scalable component still holds back the entire code," says Glosli. "In our analogy, it's like having a truck in every lane." By assigning parts of a calculation to different processors—in essence, limiting trucks to just a few lanes—the team developed an approach for parallelization that allows multiple force terms to be computed concurrently. The overall calculation now scales effectively across hundreds of thousands of processors, maximizing the power of Dawn. The team was recognized as a 2009 Gordon Bell Prize finalist for developing this strategy.

"The heterogeneous decomposition of the computational problem and optimal mapping to hardware has far-reaching implications for scientific computing," notes Glosli. "It likely will affect the way future computer codes are developed for massively parallel environments." The flexibility of this approach allows more complicated models to be developed, and the technique can be applied on current and next-generation machines. The team has also developed methods to include shorter-range physical processes, such as radiation, recombination, ionization, and fusion, in the code. Says Streitz, "Our goal for this project is to deliver a comprehensive simulation tool for computing correlations and transport properties in burning plasma."

—Katie Walter

Key Words: Dawn, Gordon Bell Prize, Institute for Scientific Computing Research (ISCR), National Ignition Facility, plasma simulation, Sequoia, Summer Visitor Program.

For further information contact Fred Streitz (925) 423-3236 (streitz1@llnl.gov).

Quickly Identifying Viable Pathogens from the Environment

THE intentional release of pathogenic viruses, bacteria, or other biological threat agents in high-traffic areas such as a busy airport or train station could have catastrophic consequences, causing widespread fear and panic in addition to quickly spreading deadly diseases. Biothreat agents can be dispersed in air, water, or food and are extremely difficult to detect and identify. They are relatively easy and inexpensive to obtain or produce, which makes them an appealing weapon for terrorists.

In the event of a biological attack or other contamination incident, laboratory technicians would need to quickly process hundreds to thousands of samples to identify the type of pathogen released and determine the extent of contamination. Clearance sampling conducted before a decontaminated site can be returned to normal operations must be sensitive enough to detect very low levels of live spores in an environment that also contains a high number of biothreat agent spores killed in the cleanup activities. Decision makers need sampling results returned quickly to minimize the time that contaminated areas are closed to the public.

Current techniques for detecting viable pathogens involve several labor- and time-intensive steps, such as pipetting, centrifuging, plating, and colony counting. In addition, laboratories can process only 30 to 40 surface samples per day with these techniques, and confirmed results can take several days to obtain.

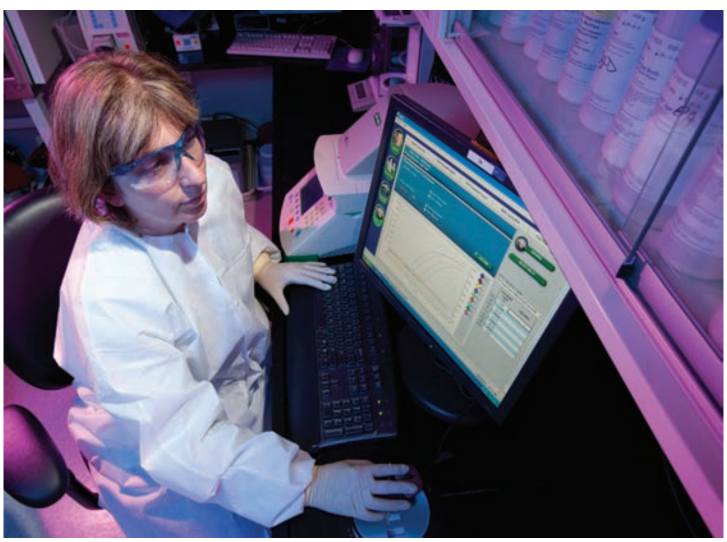
Livermore scientists (from left) Gloria Murphy and Teneile Alfaro demonstrate the automated processing of environmental samples using rapid viability polymerase chain reaction (RV-PCR).

To mitigate these efficiency issues, microbiologist Staci Kane and materials scientist Sonia Létant of Livermore's Physical and Life Sciences Directorate are developing a procedure to analyze samples and identify viable pathogens in less than 15 hours—significantly faster than the current process. Their method uses polymerase chain reaction (PCR) to amplify specific DNA sequences before and after culturing, and it can detect quantities as small as a few spores or cells of a deadly biothreat agent. Called rapid viability PCR (RV-PCR), this technique can efficiently distinguish viable spores or cells from dead ones and nonvirulent bacterial strains from virulent strains with the same level of confidence as provided with the traditional approach.

Kane and Létant are also developing robotic techniques to decrease the risk of human exposure to pathogens and increase the number of samples that can be tested at once. Livermore scientists have verified these new techniques using samples spiked with select bioagents and other contaminants, such as dirt, that could be present in specimens collected in the field. "With lab robotics, hundreds of surface samples could be processed per day with confirmed results reported the next day," says Kane, who leads the method development effort for the Laboratory's Interagency Biological Restoration Demonstration.

Technological Challenges for a Quick Assessment

The need for faster identification methods became clear following the 2001 anthrax attacks on several U.S. Postal Service buildings and the Hart Senate Office Building. Contaminated facilities remained closed for months while response teams worked to decontaminate them. To improve the nation's response capabilities, the Department of Homeland Security funded several projects to shorten the time needed to restore a site following a bioattack.



Sonia Létant, a materials scientist in the Laboratory's Physical and Life Sciences Directorate, reviews results produced on samples analyzed with Livermore's RV-PCR technique.

One of these projects is adapting the RV-PCR process to more quickly detect and assess the viability of *Bacillus anthracis*, the Gram-positive, endospore-forming bacteria that cause anthrax. Endospores are dormant, highly resistant structures that can survive extreme environmental stresses such as high temperature, high ultraviolet irradiation, desiccation, and chemical damage, which would normally kill the bacterium. Because of these extraordinary resistance properties, endospores are not readily killed by antimicrobial treatments and thus are of particular concern in decontamination scenarios.

In the Homeland Security project, the Livermore team is developing high-throughput sample processing to detect live *B. anthracis* surrogates in various environmental samples, including wipes, swabs, air filters, vacuum filters, vegetation, and soil. The Environmental Protection Agency (EPA) is supporting a related effort to optimize the technique and verify its ability to detect virulent agents.

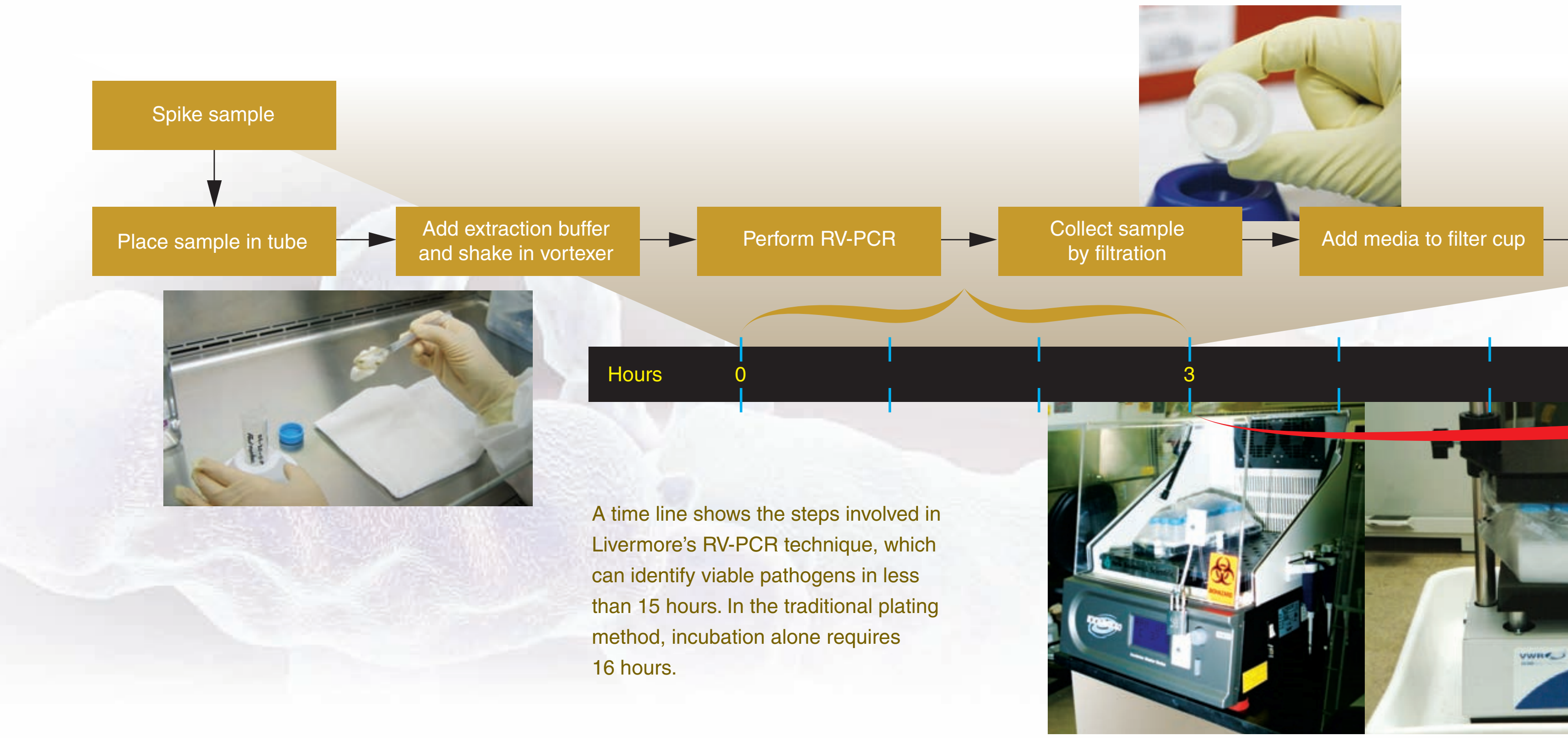
"A key part of the risk assessment after an attack is to determine whether living bioagent spores are present," says Kane. The RV-PCR approach would reduce the time for such assessments, so cleanup activities could be completed more quickly. "Our goal is to validate RV-PCR and get it deployed to the response community," Kane adds. "Our technique could ultimately be adopted by the EPA Environmental Response Laboratory Network for use following a bioagent release."

A Shorter Process with Better Results

Incubating a sample is a critical part of Kane and Létant's technique. By comparing the PCR results before and after incubation, they can determine whether bioagent spores or cells are dead or alive. "If everything is dead, no new DNA will be produced," says Létant, who is leading a team of five researchers for the EPA effort. "The change in PCR response shows us whether viable spores or cells are present."

Part of the EPA project was dedicated to choosing the optimal PCR assays for *B. anthracis*. The requirements for effective assays include selectivity, sensitivity, and robustness. The Livermore bioinformatics group, led by computer scientist Tom Slezak, used computational techniques to analyze assays from multiple sources. Létant and her team evaluated the top 10 assays and ultimately selected three—one for the *B. anthracis* chromosome and one for each of its plasmids. These assays had sensitivities below 10 genome copies, they were selective, and they were not affected by the presence of growth medium and cell debris in the PCR reaction.

With the RV-PCR method, samples such as surface wipes, air filters, water, and soil are placed in tubes and sent to a laboratory



A time line shows the steps involved in Livermore's RV-PCR technique, which can identify viable pathogens in less than 15 hours. In the traditional plating method, incubation alone requires 16 hours.

for processing, either manually by trained laboratory personnel or mechanically by a robotic platform. The technician (or robot) adds an extraction buffer to the sample inside the tube, and a machine called a vortexer shakes the tube, which releases spores from the sample material into the buffer solution. The sample is then transferred to a cup with a filter that collects the released spores. The filter is washed to remove contaminants, and growth medium is added to the sample. A portion of the mixture is withdrawn to serve as a baseline. The remainder is transferred to an incubator for 9 hours. After incubation, a second PCR sample is withdrawn.

All of these samples, or aliquots, undergo a chemical process called lysing, which ruptures a cell membrane to release the cell's DNA. Samples are then magnetically "cleaned" to remove the remaining debris and concentrate the spores' DNA. Only germinated spores and resulting cells respond to the lysing process, so DNA from dead or intact spores is not detected. "The concentration of DNA increases with the number of live *B. anthracis* cells in the sample," says Létant.

Improving on the Standard Approach

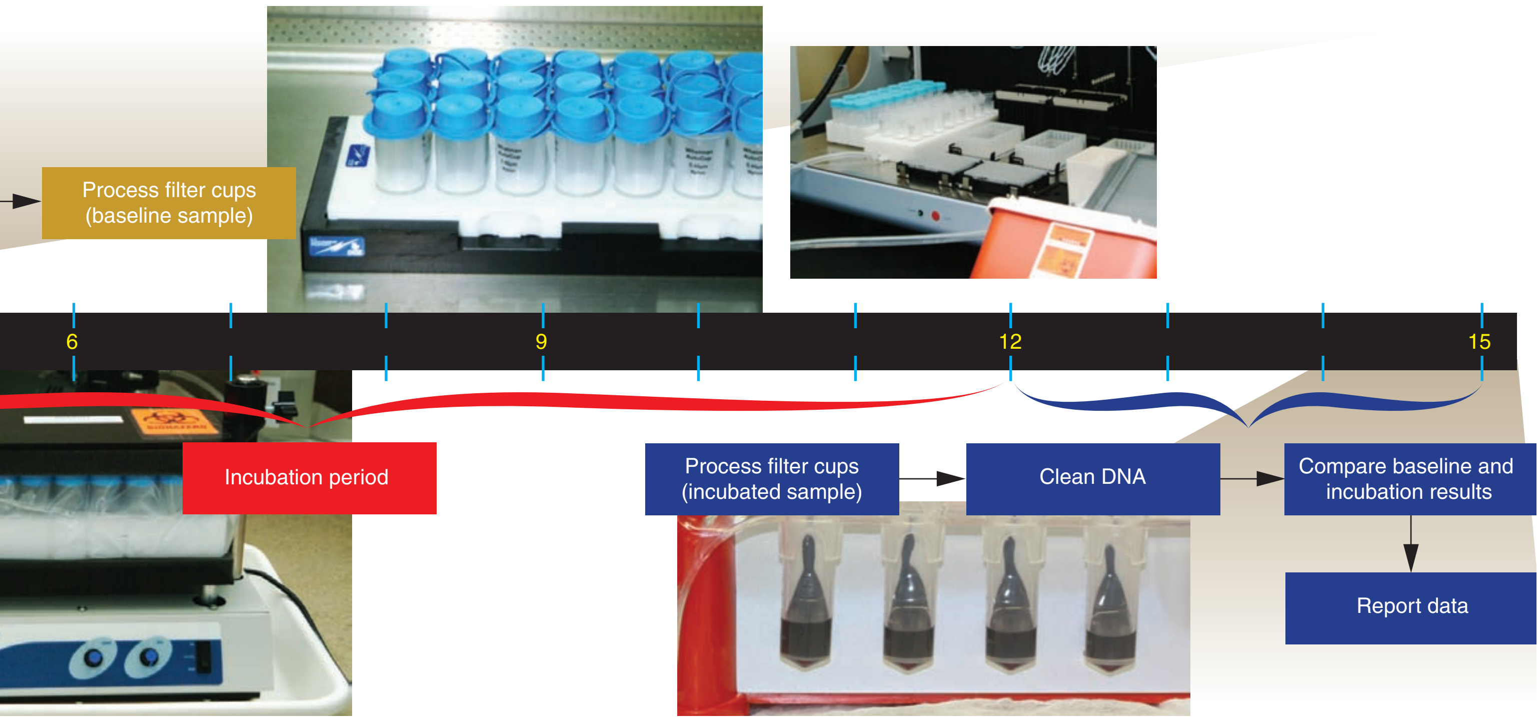
The current standard for identifying viable biothreat agents is the plating method. With this technique, cells are grown in a Petri dish on solid media containing nutrients. The plating method requires additional steps to prepare the samples and to confirm the results. Because this method is not as sensitive as PCR analysis, samples must be incubated for 16 hours or more to grow enough cells for detection. By comparison, RV-PCR can determine pathogen viability after only 9 hours of incubation time. The plating method also takes several days to confirm those initial results, whereas the RV-PCR approach generates confirmed results in 15 hours.

Detecting *B. anthracis* colonies in a sample containing an abundance of other bacterial colonies can be a challenge with the plating method. "Plates can be overwhelmed by growth from organisms that are naturally present in the environment," says Létant. "The RV-PCR method is selective and can detect the organism of interest in a very high background of other live organisms." RV-PCR also allows technicians to analyze a larger portion of the sample and to detect smaller concentrations of spores than they can with plating.

In the automated version of the RV-PCR method, a robot performs the liquid-handling steps, including mixing and transferring buffer-sample extracts to filtration cups for spore collection, washing filters, adding growth medium to the filter cups for culturing, and sampling cultures for PCR analysis. Using robots is more accurate and less time-consuming than the manual operation. In addition, the automated process is safer because it reduces a technician's risk of exposure to deadly pathogens.

Testing the Technique

To test the accuracy and speed of the RV-PCR method, the team conducted a laboratory verification study designed to evaluate various scenarios, including decontamination. In this experiment,



the team processed 200 samples, including wipes, air filters, and water—all spiked with live, virulent *B. anthracis* spores. The samples, which were divided into eight batches, also contained contaminants ranging from dirt and debris to live, nontarget spores and microorganisms and dead *B. anthracis* spores. "Including positive and negative controls ensures that no cross-contamination occurs during analysis," says Kane.

The RV-PCR method processes the first batch in under 15 hours, consistently detecting at a level of 10 or more spores per sample—one order of magnitude below the detection limit demonstrated by the traditional plating method. However, says Létant, "When hundreds of samples are processed, each batch after the first one adds 3 hours to the turnaround time for results."

The Livermore team also tested a variation of the new technique, called most-probable-number RV-PCR, using *B. anthracis* surrogates and compared the results with those from the traditional culture method. This test was designed to quantitatively estimate the *B. anthracis* spore levels in various sample types generated by the Centers for Disease Control and Prevention in a national validation study of the plating method. In the comparison tests, most-probable-number RV-PCR accurately identified all the samples in less than 24 hours, and the number of spores it detected was within the same order of magnitude as the traditional culture method.

An exercise conducted at the San Francisco International Airport in January 2006 demonstrated how the RV-PCR technique could be used in a bioattack scenario. In July 2010, a Seattle demonstration deployed RV-PCR inside a semitruck set up as a mobile laboratory. Called the Biothreat Response Vehicle, the truck contains robotics, PCR equipment, and biosafety cabinets for processing samples.

"Time is of the essence in responding to a bioattack," says Thomas Bunt, a program leader in Livermore's Global Security Principal Directorate. "The nation has a critical need for fast analysis methods and mobile laboratories, not only to characterize the extent of an attack but also to verify that decontamination efforts have cleared facilities for normal operations. Tools such as RV-PCR and the Biothreat Response Vehicle are valuable assets, protecting the public from exposure to deadly biothreat agents."

—*Kristen Light*

Key Words: anthrax, *Bacillus anthracis*, biological threat agent, bioterrorism, pathogen, rapid viability polymerase chain reaction (RV-PCR), spore.

For further information contact Staci Kane (925) 422-7897 (kane11@llnl.gov) or Sonia Létant (925) 423-9885 (letant1@llnl.gov).

A Discriminating Device to Detect Antineutrinos

Inside a nuclear reactor such as the Advanced Test Reactor at Idaho National Laboratory, Cerenkov radiation (the blue glow) is produced as part of the fission processes occurring within the reactor core. This same radiation could be useful in detecting antineutrinos. (Courtesy of Idaho National Laboratory.)

INSIDE a nuclear reactor, as uranium and plutonium undergo fission, an eerie, blue glow emanates from the reactor core. Called Cerenkov radiation, this light is produced when charged particles travel faster than the speed of light within a dielectric (nonconductive) material, such as water, whose refraction index reduces the light's speed from what it would be in a vacuum. Cerenkov radiation is typically used to measure the intensity of the fission processes within a reactor. Now, it has also become the basis for an antineutrino detector designed to improve monitoring capabilities at nuclear facilities and enhance international nonproliferation efforts.

With funding from the National Nuclear Security Administration's Office of Nonproliferation and Verification Research and Development, scientists at Lawrence Livermore and Sandia national laboratories in California have been working together for years to build antineutrino detectors for national security applications. Previous prototypes used scintillator materials to detect these elementary particles and had to be located underground in an area near a reactor's core. (See *S&TR*, July/August 2008, pp. 23–25.) Although the devices were effective, not all reactors have underground galleries near their cores, which limits the number of sites where those detectors could be deployed.

A new water-based detector designed to operate aboveground would be easier to install than underground scintillator detectors and would reduce the environmental impact. "We designed the water-based detector based in part on feedback we received from IAEA [the International Atomic Energy Agency]," says Livermore physicist Adam Bernstein, who leads the project team. "IAEA wanted a device that could be shipped to a reactor site and easily positioned for monitoring. Our sponsors agreed that this would be a useful advance in the technology."

IAEA is the world's watchdog for monitoring nuclear reactors to ensure that nuclear materials in the reactor core are not diverted for use in weapons. By detecting antineutrinos—a natural by-product of the fission of uranium-235 and plutonium-239 within a reactor core—authorities can accurately monitor a reactor's thermal power and fissile inventory and determine if further facility inspections are needed. (See *S&TR*, January/February 2006, pp. 21–23.) An aboveground antineutrino detector could be more efficient than the underground technology for determining whether nefarious activities are afoot.

The Antineutrino Two-Step

Detecting antineutrinos is a tricky business, partly because of their elusive nature. These nearly massless, uncharged particles have a low interaction probability. That is, they can travel hundreds of thousands of kilometers without ever interacting with matter. Researchers can compensate for the low interaction probability by taking advantage of the huge flux of antineutrinos that pass through detectors located a few tens of meters from a reactor's core. Tests using prototype devices reliably measured a few hundred interactions per day—an event rate high enough to accurately predict whether a reactor is operating under normal conditions.

The antineutrino signal produced within a scintillator detector consists of two bright flashes of light that occur almost simultaneously, just a few tens of microseconds apart. Initial prototype detectors used scintillator doped with gadolinium to enhance this two-step signal. When an antineutrino collides with one of the many protons available within the scintillator–gadolinium mixture, it produces a positron and a neutron. The positron soaks up most of the antineutrino's energy and creates a flash of light as it travels through the medium, before rapidly annihilating on an electron. The neutron loses energy as it bounces off protons in the scintillator, until it is absorbed by a gadolinium nucleus about 30 microseconds after the positron flash.

The captured neutron puts the nucleus into an excited quantum state, from which it immediately decays, giving off gamma rays. The gamma rays transfer energy to electrons, which then scintillate as they move through the medium, creating the second flash of light. Photomultiplier tubes detect the light from both flashes, and computer software analyzes and stores the information.

Detectors with a vat of homogenous scintillation fluid require a substantial amount of shielding, such as lead or polyethylene, as well as rock overburden to protect the material from background radiation in the environment, such as high-energy neutron radiation induced by cosmic muons. These particles rain down on the detector and mimic the antineutrino signal. "One challenge to building an aboveground detector was figuring out how to reduce the cosmic-ray-induced neutron background," says Bernstein. "By using water instead of scintillator fluid, we've built a detector that may be able to do just that."

A Need for Speed

The water-based detector creates antineutrino signals in much the same way that scintillator detectors do. However, instead of creating scintillation light, the positron and neutron produce weaker but still detectable flashes of Cerenkov light. The first blue flash is created by the positron as it moves faster than the speed of light through the water–gadolinium mixture. A gadolinium nucleus captures the neutron, creating a cascade of gamma rays, which then generate fast Compton-scattered electrons that produce the second flash of Cerenkov light.

"We first considered doping water with gadolinium about 10 years ago to build detectors for identifying antineutrino bursts from nuclear explosions," says Bernstein. "We had to shelve the concept because at the time the detectors would have been too big to deploy. The nonproliferation community became interested in the technology when more recent tests showed that small aboveground devices could reject background radiation, so we began to work on the idea again."

Water has a potential advantage over scintillator fluid for an aboveground detector because water makes the detector impervious to background radiation produced from high-energy neutrons. These cosmic particles are common at the surface of Earth and are the main source of background in scintillator detectors. When high-energy neutrons collide with protons in a scintillation mixture, the protons recoil, generating scintillation pulses. This interaction slows down the neutron, causing it to undergo neutron capture and produce another pulse of light. The two bright pulses occurring close in time are detected by the photomultiplier tubes and are recorded as if they were an antineutrino's signal.

Livermore postdoctoral researcher Greg Keefer (left) carefully cleans the interior surfaces of a shell for a prototype antineutrino detector prior to installing other components. Dust or dirt could cloud the water and decrease the antineutrino signal strength. Laboratory physicist Steve Dazeley (right) assembles a photomultiplier tube array at the top of the prototype. Without shielding, the entire detector measures about 1 cubic meter.

The antineutrino detector fits inside a standard cargo container (right) along with the electronics needed to record, analyze, and store data. The detector was built at Livermore and assembled in its shield at Sandia National Laboratories, California, before being transported in the container to the San Onofre Nuclear Generating Station (background) for testing.

In water, the high-energy neutron hits the proton, and the proton recoils. However, the proton does not have enough speed to reach above the threshold for producing Cerenkov light. "A proton is about 2,000 times heavier than an electron, which makes it difficult to budge," says Bernstein. "Most neutrons near Earth's surface just don't have the energy to induce proton recoil velocities greater than the speed of light, so the Cerenkov flash is never generated." As a result, only one flash is produced when the captured neutron creates the familiar gamma-ray cascade, so the event is rejected. Because the water-based detector effectively eliminates the signal from high-energy neutrons, it requires far less overburden shielding and thus should function well aboveground.

A Perfect Match

The antineutrino detector effort builds on the Livermore–Sandia team's pioneering studies of antineutrino-based monitoring applications as well as research into dark matter and other basic nuclear and atomic science, including neutrino oscillations. (See *S&TR*, April 2003, pp. 13–19.) Bernstein adds that the team's work reflects a natural synergy between fundamental experimental science and the multifaceted nonproliferation programs at the national laboratories. In addition to Bernstein, the team includes Nathaniel Bowden, Steve Dazeley, and Greg Keefer at Livermore and Dave Reyna, Scot Kiff, Jim Brennan, Jim Lund, and Belkis Cabrera-Palmer at Sandia/California.

The Livermore–Sandia team recently deployed a prototype aboveground detector at the San Onofre Nuclear Generating Station in southern California, where the underground prototypes were installed. For the next several months, the detector will undergo testing to determine its accuracy and overall effectiveness. "We'll need three to six months to demonstrate that we have a stable, antineutrinolike signal," says Bernstein. "Ironically, the best evidence for the existence of that signal is when the reactor is shut down, which should reduce the antineutrinolike event rate. If the signal drops by a statistically significant amount, we can have high confidence that we are actually registering reactor antineutrinos."

The next reactor shutdown at San Onofre is scheduled for the end of 2010. Team members will operate the prototype through the shutdown and check for the change in the measured antineutrino rate. In addition, they will use other analysis methods and data checks to ensure that they are tracking antineutrinos rather than reactor-generated gamma rays or neutrons. "This test would represent a first-ever demonstration of the concept," says Bernstein. "We'll need to perform additional testing and extensive evaluations before a working detector can be deployed by an agency such as IAEA." Ultimately, the automated device could make monitoring nuclear reactors easier, less time consuming for personnel, and more cost effective.

And other detectors are in the works. "New designs will focus on reducing a detector's footprint from the size of a standard office to that of a small table," he says. The team is also working with industrial partners to develop water-based neutron detectors for other national security applications. By furthering their understanding of the smallest building blocks of the universe, scientists are improving the nation's security one antineutrino at a time.

—*Caryn Meissner*

Key Words: aboveground antineutrino detector, Cerenkov light, International Atomic Energy Agency (IAEA), nonproliferation, nuclear reactor, San Onofre Nuclear Generating Station, scintillator.

For further information contact Adam Bernstein (925) 422-5918 (bernstein3@llnl.gov).

Patents and Awards

In this section, we list recent patents issued to and awards received by Laboratory employees. Our goal is to showcase the distinguished scientific and technical achievements of our employees as well as to indicate the scale and scope of the work done at the Laboratory.

Patents

Explosively Driven Low-Density Foams and Powders

James A. Viecelli, Lowell L. Wood, Muriel Y. Ishikawa, John H. Nuckolls, Philip F. Pagoria
U.S. Patent 7,707,819 B2
May 4, 2010
A Comp B booster initiated hollow RX-08HD cylindrical charges loaded with boron and polytetrafluoroethylene (PTFE) in the form of low-bulk-density powders or powders dispersed in a rigid foam matrix. The resulting detonation wave propagated the length of the cylinder, crushing the foam or bulk powder and collapsing the void spaces. Crushing the material heated it to high temperature and expelled it in a high-velocity fluid jet. In experiments with boron particles supported in foam, framing camera photos, temperature measurements, and aluminum witness plates indicate that the boron was completely vaporized by the crush wave and that the boron vapor turbulently mixed with and burned in the surrounding air. With the PTFE powder, x-ray photoelectron spectroscopy of residues recovered from fragments of a granite target slab show that heating dissociated the PTFE to carbon vapor and molecular fluorine, which reacted with the quartz and aluminum silicates in the granite to form aluminum oxide and mineral fluoride compounds.

Imaging Mass Spectrometer with Mass Tags

James S. Felton, Kuang Jen J. Wu, Mark G. Knize, Kristen S. Kulp, Joe W. Gray
U.S. Patent 7,728,287 B2
June 1, 2010
This method for analyzing biological material exposes the sample to a recognition element coupled to a mass tag element. The ion beam of a mass spectrometer directed toward the biological material interrogates at least one region of the material. The system then distributes the produced data in plots.

Bonded Polyimide Fuel Cell Package

Jeffrey D. Morse, Alan Jankowski, Robert T. Graff, Kerry Bettencourt
U.S. Patent 7,732,086 B2
June 8, 2010
In this process for fabricating microfluidic fuel-cell systems with embedded components, micrometer-scale features are formed by bonding layers of DuPont Kapton® polyimide laminate.

Hand-Held, Mechanically Cooled, Radiation Detection System for Gamma-Ray Spectroscopy

Morgan Thomas Burks, Joel Del Eckels
U.S. Patent 7,732,781 B2
June 8, 2010
This system has a radiation detector surrounded by two enclosures. The first enclosure includes a low-emissivity infrared reflective coating to thermally isolate the detector. This first enclosure is suspension-mounted to a second enclosure so that a device for cooling the detector is coupled to the first enclosure via a cooling interface positioned on the second enclosure. A second cooling interface on the second enclosure allows another cooler separate from the radiation detection system to be coupled to the first enclosure. Other setup designs can also be implemented.

Shape Memory Polymer Medical Device

Duncan Maitland, William J. Benett, Jane P. Bearinger, Thomas S. Wilson, Ward Small IV, Daniel L. Schumann, Wayne A. Jensen, Jason M. Ortega, John E. Marion III, Jeffrey M. Loge
U.S. Patent 7,744,604 B2
June 29, 2010
A system for removing matter from a conduit includes steps for passing a transport vehicle and a shape memory polymer material through the conduit. Energy transmitted to the polymer transforms it from its first shape to a second shape. The system can then withdraw the transport vehicle and the shape memory polymer through the conduit carrying the matter to be removed.

Catalyst for Microelectromechanical Systems Microreactors

Jeffrey D. Morse, David A. Sopchak, Ravindra S. Upadhye, John G. Reynolds, Joseph H. Satcher, Alex E. Gash
U.S. Patent 7,744,830 B2
June 29, 2010
This microreactor has a silicon wafer with several microchannels and a catalyst for coating the microchannels. The catalyst can be a nanostructured material, an aerogel, a solgel, or carbon nanotubes.

System for Analysis of Explosives

Jeffrey S. Haas
U.S. Patent 7,745,227 B2
June 29, 2010
In this system for analyzing explosives, samples of multicomponent explosives standards are placed on a thin-layer chromatography plate. The plate is dipped in a solvent mixture, and chromatography is allowed to proceed. The plate is dipped in a reagent, heated, and then dipped in a second reagent.

Lipid Nanotube or Nanowire Sensor

Aleksandr Noy, Olgica Bakajin, Sonia Létant, Michael Stadermann, Alexander B. Artyukhin
U.S. Patent 7,745,856 B2
June 29, 2010
This sensor apparatus has a nanotube or nanowire, a lipid bilayer around the nanotube or nanowire, and a sensing element connected to the lipid bilayer. Another biosensor apparatus includes gate, source, and drain electrodes; a nanotube or nanowire connected to each electrode; a lipid bilayer around the nanotube or nanowire; and a sensing element connected to the lipid bilayer.

Awards

Livermore physicist **Natalia Zaitseva** of the Physical and Life Sciences Directorate received the **R. A. Laudise Prize** from the **International Organization for Crystal Growth** (IOCG) for her work on "creating the technology and scientific basis of rapid growth of perfect crystals from solutions." IOCG, an international federation of regional and national groups and societies, is dedicated to the advancement of the theory and practice of crystal growth, crystal characterization, and allied branches of science. Every three years, it awards the R. A. Laudise Prize for "significant technological contributions to the field of crystal growth."

The **Department of Energy** (DOE) honored 16 Laboratory researchers with the **2009 Outstanding Mentor Award** for their work with students in the summer of 2009. The recipients are as follows: **Adam Bernstein**, **Kareem Kazkaz**, **Dawn Shaughnessy**, **Roger Henderson**, **Christine Orme**, **Amy Gaffney**, **Trevor Willey**, and **Roger Qiu** from the Physical and Life Sciences Directorate; **Jeff Westcott**, **Gary Laguna**, and **Tina Eliassi-Rad** from the Computation Directorate; **Klint Rose** from the Engineering Directorate; **Steve Langer** and **Robert Rieben** from the Weapons and Complex Integration Principal Directorate; **Zafer Demir** from the Operations and Business Principal Directorate; and **Phil Burger** from the Office of Independent Audit and Oversight.

DOE established the Outstanding Mentor Award in 2002 to foster a complexwide culture that values mentorship. The award program is coordinated through the Office of Science Workforce Development for Teachers and Scientists.

Abstract

Science in Support of International Weapon Treaties

For more than five decades, Lawrence Livermore scientists have helped support international weapon treaties and agreements. Livermore experts have provided guidance on specific treaty wording, developed verification technologies, and helped international organizations ensure compliance. The Laboratory has applied its nuclear weapons expertise to the challenge of nuclear nonproliferation through support of the International Atomic Energy Agency (IAEA) and the Nuclear Non-Proliferation Treaty, which limits the spread of nuclear weapons and their materials. To help strengthen IAEA verification technologies and scientific resources, staff members are participating in the Department of Energy's 2009 Next Generation Safeguards Initiative. In addition, the Forensic Science Center provides technical support to the Organisation for the Prohibition of Chemical Weapons, which is responsible for implementing verification activities for the Chemical Weapons Convention. Laboratory personnel have also contributed to U.S. efforts to secure a Comprehensive Nuclear-Test-Ban Treaty, which bans all nuclear tests, and have provided expertise in support of the U.S. delegation negotiating the New Strategic Arms Reduction Treaty with Russia, which was signed this year.

Contact: Jay Zucca (925) 422-4895 (zucca2@llnl.gov).

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Six Award-Winning Technologies

Livermore researchers win six awards in *R&D Magazine*'s annual competition:

- GATOR: Grating-Actuated Transient Optical Recorder
- High-Performance Strontium Iodide Scintillator for Gamma-Ray Spectroscopy
- Microelectromechanical-Systems-Based Adaptive-Optics Optical Coherence Tomography
- SRaDS: Statistical Radiation Detection System
- Ultrapermeable Carbon Nanotube Membranes
- X-Ray Free Electron Laser Energy Monitor

Also in October/November

• A 21-year partnership between Livermore and a Russian nuclear physics institute has added the six heaviest elements to the periodic table.

• Competitive summer internships pair Laboratory researchers with students for hands-on career experience.

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